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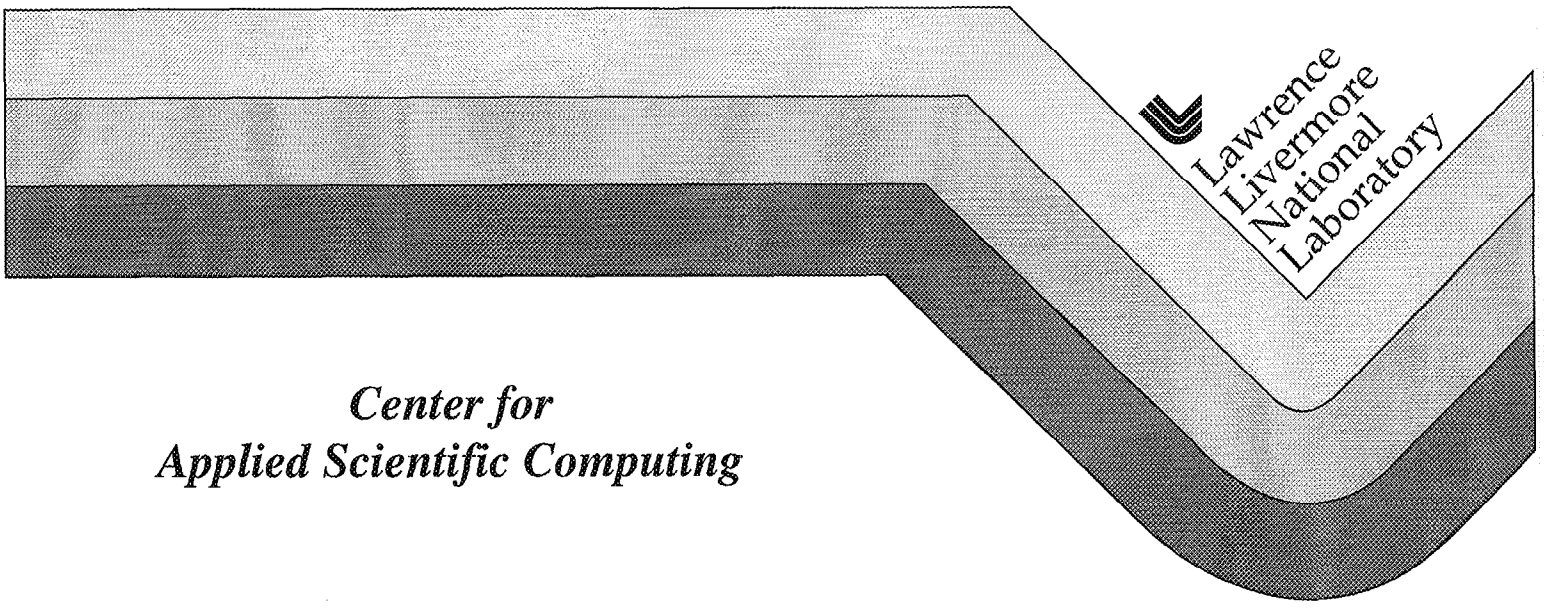

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ON THE USE OF DIFFUSION SYNTHETIC ACCELERATION IN PARALLEL 3D NEUTRAL PARTICLE TRANSPORT CALCULATIONS*

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The linear Boltzmann transport equation (BTE) is an integro-differential equation arising in deterministic models of neutral and charged particle transport. In slab (one-dimensional Cartesian) geometry and certain higher-dimensional cases, *Diffusion Synthetic Acceleration* (DSA) is known to be an effective algorithm for the iterative solution of the discretized BTE. Fourier and asymptotic analyses have been applied to various idealizations (e.g., problems on infinite domains with constant coefficients) to obtain sharp bounds on the convergence rate of DSA in such cases.

While DSA has been shown to be a highly effective acceleration (or preconditioning) technique in one-dimensional problems, it has been observed to be less effective in higher dimensions. This is due in part to the expense of solving the related diffusion linear system. We investigate here the effectiveness of a parallel semicoarsening multigrid (SMG) solution approach to DSA preconditioning in several three dimensional problems. In particular, we consider the algorithmic and implementation scalability of a parallel SMG-DSA preconditioner on several types of test problems.

The Boltzmann Equation. We begin with the linear time-dependent BTE in a three dimensional box geometry with general scattering [8]. The spatial domain is the box $\mathcal{D} \equiv \{r = (x,y,z) | a_x \le x \le b_x, a_y \le y \le b_y,$ and $a_z \le z \le b_z\}$, the direction variable is $\Omega \in \mathcal{S}^2$, the unit sphere in $\mathbf{R}^3$, the energy variable is $E \in (0,\infty)$, the time variable is t, and the equation in the flux $\psi(r,\Omega,E,t)$ is given by

$$\begin{aligned} &\frac{1}{v(E)}\frac{\partial}{\partial t}\psi(r,\Omega,E,t) + \Omega\cdot\nabla\psi(r,\Omega,E,t) + \sigma(r,E)\psi(r\Omega,E,t) \\ &= \int_0^\infty \int_{\mathcal{S}^2} \psi(r,\Omega',E',t)\sigma_s(r,\Omega'\cdot\Omega,E'\to E)d\Omega' dE' + q(r,\Omega,E,t), \end{aligned} \tag{1}$$

where $\nabla\psi \equiv (\partial\psi/\partial x, \partial\psi/\partial y, \partial\psi/\partial z)$ and $v(E)$ is the particle speed. The energy variable E is discretized into energy subgroups, giving rise to a linear system that is blocked by energy group. When using implicit time integration methods, a linear system of this form must be solved at each timestep, usually via a block Jacobi solution method. To invert the block diagonal of this matrix a sequence of mono-energetic, steady-state problems of the general form

$$\Omega\cdot\nabla\psi(r,\Omega) + \sigma(r)\psi = \int_{\mathcal{S}^2} \psi(r,\Omega')\sigma_s(r,\Omega'\cdot\Omega)d\Omega' + q(r,\Omega), \tag{2}$$

must be solved for each energy group at each timestep. Thus, in what follows we concentrate on the solution of (2).

When solving (2), the flux $\psi(r,\Omega)$ is expanded in surface harmonics according to

$$\psi(r,\Omega) = \sum_{n=0}^{\infty}\sum_{m=-n}^{n} \phi_n^m(r) Y_n^m(\Omega),$$

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where $Y_n^m(\Omega)$ is a surface harmonic and

$$\phi_n^m(r) \equiv \int_{\mathcal{S}^2} \psi(r,\Omega) Y_n^m(\Omega) d\Omega$$

is the $(n,m)^{th}$ moment of ψ. The source q is similarly expanded.

Given ψ in the above form, one is able to rewrite the scattering integral in the form

$$\int_{\mathcal{S}^2} \sigma_s(r, \Omega' \cdot \Omega)\psi(r,\Omega')d\Omega' = \sum_{n=0}^{\infty} \sigma_{s,n}(r) \sum_{m=-n}^{n} \phi_n^m(r) Y_n^m(\Omega), \tag{3}$$

where the $\sigma_{s,n}$ are given by

$$\sigma_{s,n}(r) \equiv 2\pi \int_{-1}^{1} \sigma_s(r,\mu_0) P_n(\mu_0) d\mu_0,$$

and where μ_0 is the cosine of the scattering angle. The total cross section σ is given by

$$\sigma(r) \equiv \sigma_a(r) + 2\pi \int_{-1}^{1} \sigma_s(r,\mu_0) d\mu_0 = \sigma_a(r) + \sigma_{s,0}(r),$$

where σ_a is the absorption cross section.

Boundary conditions must also be specified so as to make (2) well-posed. Various options include a reflecting condition on a face, or a Dirichlet condition in which the incident flux is specified on a face. For simplicity, we will consider only the latter case. Namely, we will consider boundary conditions of the form

$$\psi(r,\Omega) = g(r,\Omega) \text{ for all } r \in \partial\mathcal{D} \text{ and } \Omega \in \mathcal{S}^2 \text{ with } \vec{n}(r) \cdot \Omega < 0, \tag{4}$$

where $\vec{n}(r)$ is the outward pointing unit normal at $r \in \partial\mathcal{D}$.

Discretization of the 3-D Problem. In previous work [1], we derived a matrix version of the well-known *diamond difference* discretization scheme for the 1-D slab problem analogous to (2)-(4). This formalism was crucial to the development and analysis of the 1-D DSA preconditioner discussed therein. We extended that development to 3-D problems in [2], and give a brief overivew here.

The specific quadrature rules we consider for approximating integrals on $\mathcal{S}^2$ employ the standard symmetry assumptions. Following Carlson and Lathrop [4], we consider quadrature rules of the form

$$\int_{\mathcal{S}^2} \psi(\Omega) d\Omega \approx \sum_{\ell=1}^{L} w_\ell \psi(\Omega_\ell), \tag{5}$$

where $\Omega_\ell \equiv (\mu_\ell, \eta_\ell, \xi_\ell)$, for all $\ell = 1, \ldots, L$, with $L = \nu(\nu+2)$ and ν is the number of direction cosines ($\nu = 2, 4, 6, \ldots$). See [2] for more details.

We use a *Petrov-Galerkin* finite-element method for the solution of the problem

$$\begin{cases} \Omega \cdot \nabla\psi + \sigma\psi = f \text{ in } \mathcal{D}, \\ \psi(r) = g(r) \text{ for all } r \in \partial\mathcal{D} \text{ with } \vec{n}(r) \cdot \Omega < 0, \end{cases} \tag{6}$$

where $\Omega = (\mu, \eta, \xi) \in \mathcal{S}^2$ is fixed and equal to one of the above quadrature points (although we suppress the ℓ subscript to simplify notation), $\mathcal{D}$ is the spatial domain defined earlier, and $\vec{n}(r)$ is the outward pointing unit normal at $r \in \partial\mathcal{D}$. The functions f, g and σ are assumed known.

We first discretize $\mathcal{D}$ into zones in the natural way, and define

$$\Delta x_i = x_i - x_{i-1} \text{ for } i = 1, \ldots, M, \quad \Delta y_j = y_j - y_{j-1} \text{ for } j = 1, \ldots, J, \text{ and}$$
$$\Delta z_k = z_k - z_{k-1} \text{ for } k = 1, \ldots, K,$$

and define $r_{ijk} = (x_i, y_j, z_k)$. Also define $\Delta r_{ijk} \equiv \Delta x_i \Delta y_j \Delta z_k$. The $\{r_{ijk}\}$ are referred to as *nodes*, and function values at these points are called *nodal values*. Assume that σ and f have constant values on each *zone*

$$\mathcal{Z}_{ijk} \equiv \{r | x_{i-1} < x < x_i, y_{j-1} < y < y_j, z_{k-1} < z < z_k\},$$

denoted by σ_{ijk} and f_{ijk}, respectively. Function values that are constant on zones will be referred to as *zone-centered* values. We use ψ_{ijk} to denote the approximation to $\psi(r_{ijk})$, the true solution at r_{ijk}. Following the development given in [2], there are $(M+1)(J+1)(K+1)$ unknowns ψ_{ijk}. There are MJK zonal equations, and $MK + JM + JK + M + J + K + 1$ boundary equations, and we note that $(M+1)(J+1)(K+1) = MJK + MK + JM + JK + M + J + K + 1$.

Writing the discretized system in matrix notation, we first have the discrete flux vector $\Psi \in \mathbf{R}^{(M+1)(J+1)(K+1)}$, defined for all nodes ordered in the natural way. Next, define diagonal matrices $\Delta x \equiv \text{diag}(\Delta x_1, \ldots, \Delta x_M)$, with Δy and Δz similarly, and define the matrices $D_M \in \mathbf{R}^{M \times (M+1)}$ and $S_M \in \mathbf{R}^{M \times (M+1)}$ by

$$D_M \equiv \begin{pmatrix} -1 & 1 & & \\ & \ddots & \ddots & \\ & & -1 & 1 \end{pmatrix} \text{ and } S_M \equiv \frac{1}{2} \begin{pmatrix} 1 & 1 & & \\ & \ddots & \ddots & \\ & & 1 & 1 \end{pmatrix}. \tag{7}$$

In a similar way, define the matrices D_J, S_J, D_K, and S_K. Let $\Sigma \equiv \text{diag}(\sigma_{111}, \ldots, \sigma_{MJK}) \in \mathbf{R}^{MJK}$, and define the matrices C_x, C_y, C_z, and S by

$$C_x \equiv S_K \otimes S_J \otimes \Delta x^{-1} D_M, \quad C_y \equiv S_K \otimes \Delta y^{-1} D_J \otimes S_M,$$
$$C_z \equiv \Delta z^{-1} D_K \otimes S_J \otimes S_M, \quad \text{and } S \equiv S_K \otimes S_J \otimes S_M.$$

The matrices C_x, C_y, and C_z represent the discretized versions of the differentiation operators $\partial/\partial x$, $\partial/\partial y$, $\partial/\partial z$, respectively, and S represents an averaging matrix taking nodal vectors into zone-centered vectors. With these definitions, it is possible to write the MJK zone-centered equations in the unknown Ψ as

$$(C + \Sigma S)\Psi = F, \tag{8}$$

where $C \equiv \mu C_x + \eta C_y + \xi C_z$, and $F \equiv (f_{ijk}) \in \mathbf{R}^{MJK}$.

To isolate the boundary values, first note that for a direction vector Ω with all its components positive, ψ satisfies a Dirichlet condition for all $r = r_{0jk}$, r_{i0k}, or r_{ij0}, i.e., for an r on any one of the three faces $x = x_0$, $y = y_0$, or $z = z_0$. For any such Ω, letting G be a vector of the same dimension as Ψ whose possibly nonzero entries are values of $g(r, \Omega)$ at all the boundary points, the discrete boundary conditions can be written as $E_{000}(\Psi - G) = 0$, where

$$E_{000} \equiv \begin{pmatrix} e_{0K}^T \otimes I_{J+1} \otimes I_{M+1} \\ (0, I_K) \otimes e_{0J}^T \otimes I_{M+1} \\ (0, I_K) \otimes (0, I_J) \otimes e_{0M}^T \end{pmatrix},$$

with the vectors e_{0J} and e_{0K} having the natural interpretations. There are different E matrices for the other possible quadrature points. In all, there are eight different E_{ijk} matrices, with $i = 0$ or M, $j = 0$ or J, and $k = 0$ or K.

At this point it is necessary to introduce the dependence of Ψ, G, and the matrix C on the quadrature point Ω. For a given $\Omega = \Omega_\ell$, the vector Ψ is really Ψ_ℓ, $G = G_\ell$, and the matrix $C = C_\ell$, for the subscript ℓ corresponding to that Ω. Then the matrix representation of the discrete version of (6) can be written as

$$H_\ell \Psi_\ell = \begin{pmatrix} F_\ell \\ B_\ell G_\ell \end{pmatrix}, \text{ where } H_\ell \equiv \begin{pmatrix} C_\ell + \Sigma S \\ B_\ell \end{pmatrix}, \tag{9}$$

with $B_\ell = E_{ijk}$ for the appropriate choice of i, j, k, and $C_\ell = \mu_\ell C_x + \eta_\ell C_y + \xi_\ell C_z$. Note that H_ℓ operates on nodal vectors.

The Discrete Ordinates Method. Continuing the matrix development of the overall discretization of the BTE, we begin by defining discretized representations of the operations of taking moments of the flux. As operators on zone-centered vectors, these are easily seen to be given by the $MJK \times LMJK$ matrices

$$L_{n,m} \equiv \left(\, w_1 Y_n^m(\Omega_1) I \;\middle|\; w_2 Y_n^m(\Omega_2) I \;\middle|\; \cdots \;\middle|\; w_L Y_n^m(\Omega_L) I \, \right). \tag{10}$$

Similarly, we define the $LMJK \times MJK$ matrices

$$L_{n,m}^+ \equiv \begin{pmatrix} Y_n^m(\Omega_1) I \\ \vdots \\ Y_n^m(\Omega_L) I \end{pmatrix}, \tag{11}$$

where $I = I_{MJK}$. We also will find it useful to define the grouped matrices L_n and L_n^+, where

$$L_n = \begin{pmatrix} L_{n,-n} \\ \vdots \\ L_{n,n} \end{pmatrix}, \text{ and } L_n^+ = \left(L_{n,-n}^+, \cdots, L_{n,n}^+ \right).$$

To represent the source term, define the zone-centered vector $Q \equiv (q_{ijk\ell}) \in \mathbf{R}^{LMJK}$, where $q_{ijk\ell} \equiv q(r_{ijk}, \Omega_\ell)$. For the boundary terms, define the block diagonal matrices B and C by

$$B \equiv \text{diag}(B_1, \ldots, B_L) \text{ and } C \equiv \text{diag}(C_1, \ldots, C_L),$$

and let

$$\begin{aligned}
\Gamma_n &\equiv I_{2n+1} \otimes \hat{\Gamma}_n, \\
&\quad \text{where } \hat{\Gamma}_n \equiv \text{diag}(\sigma_{s,n,111}/\sigma_{111}, \ldots, \sigma_{s,n,MJK}/\sigma_{MJK}), \quad n = 0, 1, \\
Z &\equiv I_L \otimes Z_0, \text{ where } Z_0 \equiv \begin{pmatrix} I_{MJK} \\ 0 \end{pmatrix} \in \mathbf{R}^{(M+1)(J+1)(K+1) \times MJK} \\
Z_b &\equiv I_L \otimes Z_1, \text{ where} \\
&\quad Z_1 \equiv \begin{pmatrix} 0 \\ I_{(M+1)(J+1)(K+1)-MJK} \end{pmatrix} \in \mathbf{R}^{(M+1)(J+1)(K+1) \times (M+1)(J+1)(K+1) - MJK} \\
\ddot{\Sigma} &\equiv I_L \otimes \Sigma, \text{ and} \\
\bar{S} &\equiv I_L \otimes S.
\end{aligned} \tag{12}$$

The matrix Z injects zone-centered vectors into the nodal vector space, and the matrix $\bar{S}$ averages nodal vectors to obtain zone-centered ones. Note that $Z^T Z = I$ and $Z^T Z_b = 0$. Using the above matrices, define the matrix H by

$$H \equiv \text{diag}(H_1, \ldots, H_L) = Z(\ddot{\Sigma}^{-1} C + \bar{S}) + Z_b B. \tag{13}$$

The matrices Z and Z_b are needed since H operates on nodal vectors, while the scattering matrix operates on zone-centered vectors. (Recall that f was assumed to be zone-centered in the development of the Petrov-Galerkin method discussed earlier.) If we assume only $N+1$ terms in the scattering operator, then the complete discretization of (2)–(4) can be written in the compact form

$$H\Psi = Z\sum_{n=0}^{N} L_n^+ \Gamma_n L_n \bar{S}\Psi + F. \tag{14}$$

with $F \equiv Z\bar{\Sigma}^{-1}Q + Z_b BG$.

We now transform (14) into an equivalent moment form. For simplicity here, assume that $N = 1$. It is shown in [2] that the matrix H is invertible. So, first multiply (14) by H^{-1}, and then by either $L_0\bar{S}$ or $L_1\bar{S}$ to give

$$\begin{aligned} L_0\bar{S}\Psi &= L_0\bar{S}H^{-1}ZL_0^+\Gamma_0 L_0\bar{S}\Psi + L_0\bar{S}H^{-1}ZL_1^+\Gamma_1 L_1\bar{S}\Psi + L_0\bar{S}H^{-1}F, \\ L_1\bar{S}\Psi &= L_1\bar{S}H^{-1}ZL_0^+\Gamma_0 L_0\bar{S}\Psi + L_1\bar{S}H^{-1}ZL_1^+\Gamma_1 L_1\bar{S}\Psi + L_1\bar{S}H^{-1}F. \end{aligned}$$

Defining $\Phi_0 = L_0\bar{S}\Psi$, $\Phi_1 = L_1\bar{S}\Psi$, $R_0 = L_0\bar{S}H^{-1}F$, $R_1 = L_1\bar{S}H^{-1}F$, and defining the rectangular matrices $K_{n,n'} = L_n\bar{S}H^{-1}ZL_{n'}^+$ for $n, n' = 0, 1$, these equations are

$$A_1\begin{pmatrix}\Phi_0\\ \Phi_1\end{pmatrix} = \begin{pmatrix}R_0\\ R_1\end{pmatrix}, \text{ with } A_1 \equiv \begin{pmatrix} I_{MJK} - K_{0,0}\Gamma_0 & -K_{0,1}\Gamma_1 \\ -K_{1,0}\Gamma_0 & I_{3MJK} - K_{1,1}\Gamma_1 \end{pmatrix}. \tag{15}$$

Once Φ_0 and Φ_1 are obtained by solving (15), Ψ is recovered by solving the equation

$$H\Psi = ZL_0^+\Gamma_0\Phi_0 + ZL_1^+\Gamma_1\Phi_1 + Z\bar{\Sigma}^{-1}Q + Z_b BG. \tag{16}$$

We note that in the above development, we are lead to a linear system to be solved for the moments Φ_0 and Φ_1, namely (15). This system has the form

$$A\Phi = R. \tag{17}$$

The development was given for $N = 1$, for which the matrix A in (17) is A_1, and its size is $4MJK$. In the case of isotropic scattering, $N = 0$, only the 0^{th} moment Φ_0 needs to be computed, and the matrix A in (17) is $A = A_0 = I - K_{0,0}\Gamma_0$, of size MJK. In general, the matrix A in (17) has the form $A = I - K\Gamma$, for suitable choices of the matrices K and Γ.

Source Iteration. The iterative solution of (17) has typically been accomplished via a simple Richardson iteration. Without preconditioning, Richardson iteration for (17) is

$$\Phi^{(k+1)} = K\Gamma\Phi^{(k)} + R, \tag{18}$$

for $k = 0, 1, \ldots$, with $\Phi^{(0)}$ being some initial guess. (We note that (18) is also referred to as *source iteration* in the literature.) The iteration (18) will converge for any initial guess since the spectral radius $\rho(K\Gamma) < 1$.

Some form of preconditioning is generally needed for thick problems. If C represents a preconditioner for A, then the preconditioned A problem becomes

$$AP(P^{-1}\Phi) = R, \tag{19}$$

and the corresponding source iteration is

$$\Theta^{(k+1)} = (I - AP)\Theta^{(k)} + R,$$

for $k = 0, 1, \ldots$, with $\Theta^{(k)} = P^{-1}\Phi^{(k)}$ and some initial guess $\Theta^{(0)}$. Of course, other more powerful iterative methods such as BICGSTAB can also be used to solve the preconditioned system (19).

DSA Preconditioning. In [2] the DSA preconditioner for the discrete problem above assuming isotropic scattering is given by

$$
\begin{aligned}
(20) \qquad P_0 &= I_{MJK} + SD_{co}^{+}S^T\Sigma\Delta r\Gamma_0, \text{ where} \\
D_{co} &\equiv S^T\Delta r\Sigma_{a,0}S + \frac{1}{3}\left(C_x^T\Delta r\Sigma_{a,1}^{-1}C_x + C_y^T\Delta r\Sigma_{a,1}^{-1}C_y + C_z^T\Delta r\Sigma_{a,1}^{-1}C_z\right) \\
&+ 2\alpha S_K^T\Delta z S_K \otimes S_J^T\Delta y S_J \otimes (e_{0M}e_{0M}^T + e_{MM}e_{MM}^T) \\
&+ 2\alpha S_K^T\Delta z S_K \otimes (e_{0J}e_{0J}^T + e_{JJ}e_{JJ}^T) \otimes S_M^T\Delta x S_M \\
&+ 2\alpha(e_{0K}e_{0K}^T + e_{KK}e_{KK}^T) \otimes S_J^T\Delta y S_J \otimes S_M^T\Delta x S_M,
\end{aligned}
$$

with $\alpha \equiv (1/4\pi)\sum_{\xi_\ell>0} w_\ell\xi_\ell$, $\Sigma_{a,0} \equiv \Sigma(I-\Gamma_0)$, $\Sigma_{a,1} \equiv \Sigma(I-\hat{\Gamma}_1)$, and $\hat{\Gamma}_1$ defined as in (12). (A related preconditioner for linearly anisotropic scattering is also derived in [2].) In (20), D_{co}^{+} refers to the pseudo-inverse of the DSA matrix D_{co}. The following facts are shown in [2]:

1. D_{co} is singular.
2. $\dim(\mathcal{N}(D_{co})) = M + J + K + 1$.
3. $\dim(\mathcal{N}(S)) = MJ + JK + MK + M + J + K + 1$.
4. $\mathcal{N}(D_{co}) \subset \mathcal{N}(S)$, $\mathcal{N}(D_{co}) \subset \mathcal{N}(C_x)$, $\mathcal{N}(D_{co}) \subset \mathcal{N}(C_y)$, etc.

While D_{co} is clearly symmetric from its form, it is singular. The 4-th fact above and the form of P_0 imply that the D_{co} linear systems to solve are always consistent, i.e., they have solutions.

Parallel Implemention Issues. The parallel solution of the discretized system (17) has been discussed at length in [5], [6] and [7]. The implementation discussed therein is parallelized in all phase space variables. To this we have added a parallel implementation of the above DSA preconditioner P_0. The linear systems involving the D_{co} matrix are not solved exactly. Rather, we use a parallel multigrid method to approximately solve these systems. Specifically, we use a parallel implementation of the Shaffer semicoarsening multigrid (SMG) method discussed in [3], and perform a V(1,0) cycle to approximate the action of D_{co}^{+} times a vector. We investigate the algorithmic scalability and scaled efficiency of the above SMG-DSA preconditioned iteration on several problems involving highly diffusive regions, sometimes coupled to very thin regions.

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